



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 02:24 PM UTC

PDB ID : 6EVE / pdb_00006eve
Title : Structure of R175A *S. cerevisiae* Fdc1 with prFMN in the iminium form
Authors : Bailey, S.S.; David, L.
Deposited on : 2017-11-01
Resolution : 2.05 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

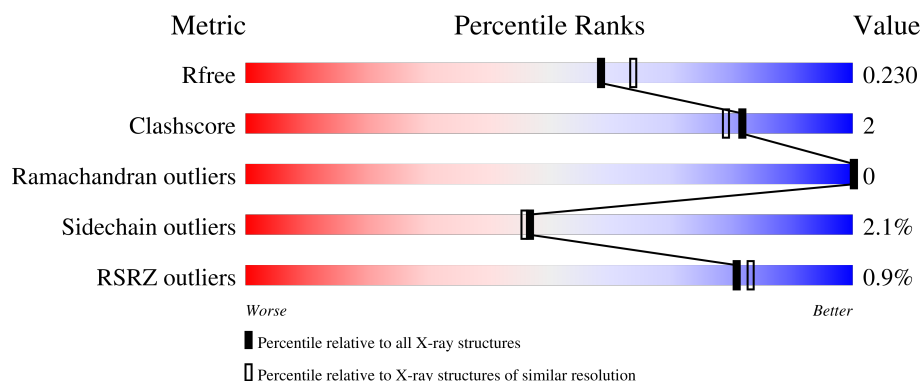
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	509	 92% 6% .
1	B	509	 91% 7% .
1	C	509	 91% 7% .
1	D	509	 90% 7% ..

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17196 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Ferulic acid decarboxylase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	500	Total	C	N	O	S	0	11	0
			3976	2558	648	745	25			
1	B	499	Total	C	N	O	S	0	9	0
			3941	2537	639	742	23			
1	C	500	Total	C	N	O	S	0	10	0
			3951	2543	642	742	24			
1	D	497	Total	C	N	O	S	0	9	0
			3931	2534	636	737	24			

There are 28 discrepancies between the modelled and reference sequences:

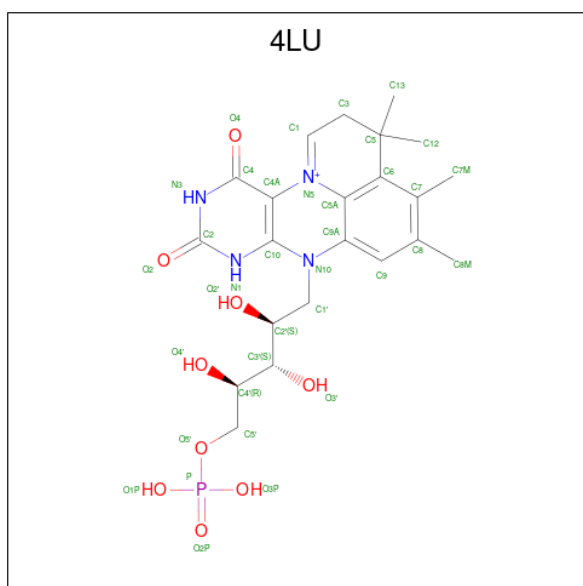
Chain	Residue	Modelled	Actual	Comment	Reference
A	175	ALA	ARG	engineered mutation	UNP Q03034
A	504	HIS	-	expression tag	UNP Q03034
A	505	HIS	-	expression tag	UNP Q03034
A	506	HIS	-	expression tag	UNP Q03034
A	507	HIS	-	expression tag	UNP Q03034
A	508	HIS	-	expression tag	UNP Q03034
A	509	HIS	-	expression tag	UNP Q03034
B	175	ALA	ARG	engineered mutation	UNP Q03034
B	504	HIS	-	expression tag	UNP Q03034
B	505	HIS	-	expression tag	UNP Q03034
B	506	HIS	-	expression tag	UNP Q03034
B	507	HIS	-	expression tag	UNP Q03034
B	508	HIS	-	expression tag	UNP Q03034
B	509	HIS	-	expression tag	UNP Q03034
C	175	ALA	ARG	engineered mutation	UNP Q03034
C	504	HIS	-	expression tag	UNP Q03034
C	505	HIS	-	expression tag	UNP Q03034
C	506	HIS	-	expression tag	UNP Q03034
C	507	HIS	-	expression tag	UNP Q03034
C	508	HIS	-	expression tag	UNP Q03034
C	509	HIS	-	expression tag	UNP Q03034

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Chain	Residue	Modelled	Actual	Comment	Reference
D	175	ALA	ARG	engineered mutation	UNP Q03034
D	504	HIS	-	expression tag	UNP Q03034
D	505	HIS	-	expression tag	UNP Q03034
D	506	HIS	-	expression tag	UNP Q03034
D	507	HIS	-	expression tag	UNP Q03034
D	508	HIS	-	expression tag	UNP Q03034
D	509	HIS	-	expression tag	UNP Q03034

- Molecule 2 is 1-deoxy-5-O-phosphono-1-(3,3,4,5-tetramethyl-9,11-dioxo-2,3,8,9,10,11-hexahydro-7H-quinolino[1,8-fg]pteridin-12-ium-7-yl)-D-ribitol (CCD ID: 4LU) (formula: $C_{22}H_{30}N_4O_9P$).



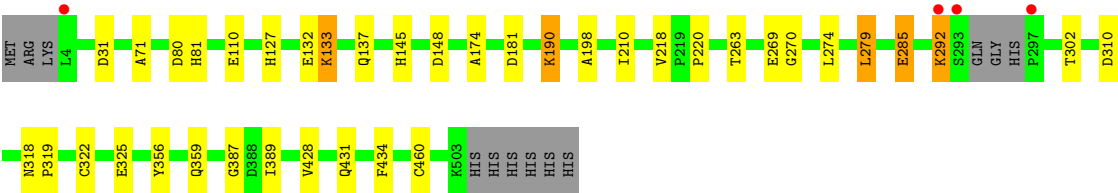
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mn 1 1	0	0
3	B	1	Total Mn 1 1	0	0
3	C	1	Total Mn 1 1	0	0
3	D	2	Total Mn 2 2	0	0

- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total K 1 1	0	0
4	B	1	Total K 1 1	0	0
4	C	1	Total K 1 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	323	Total O 323 323	0	0
5	B	317	Total O 317 317	0	0
5	C	356	Total O 356 356	0	0
5	D	249	Total O 249 249	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	117.48Å 98.64Å 118.17Å 90.00° 97.24° 90.00°	Depositor
Resolution (Å)	77.89 – 2.05 77.89 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.7 (77.89-2.05) 99.7 (77.89-2.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.183 , 0.226 0.191 , 0.230	Depositor DCC
R_{free} test set	8336 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	25.2	Xtriage
Anisotropy	0.639	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 30.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.015 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17196	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 4LU, K, MN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.19	3/4074 (0.1%)	1.10	6/5534 (0.1%)
1	B	1.35	12/4039 (0.3%)	1.15	8/5490 (0.1%)
1	C	1.16	2/4051 (0.0%)	1.11	3/5512 (0.1%)
1	D	1.17	5/4029 (0.1%)	1.09	4/5477 (0.1%)
All	All	1.22	22/16193 (0.1%)	1.11	21/22013 (0.1%)

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	280	GLU	N-CA	-20.18	1.21	1.45
1	B	285	GLU	N-CA	-19.05	1.17	1.46
1	B	175	ALA	CA-C	-16.05	1.31	1.52
1	B	175	ALA	N-CA	-15.38	1.26	1.46
1	A	5	ASN	CA-C	6.33	1.59	1.52
1	B	280	GLU	CA-C	-6.17	1.45	1.52
1	B	292	LYS	N-CA	6.10	1.54	1.46
1	B	393	THR	C-O	5.89	1.31	1.23
1	B	174	ALA	N-CA	5.73	1.53	1.45
1	A	292	LYS	N-CA	5.70	1.53	1.46
1	D	292	LYS	N-CA	5.56	1.53	1.46
1	B	229	PRO	CA-C	5.43	1.57	1.52
1	B	121	SER	CA-C	5.41	1.60	1.52
1	D	218	VAL	CA-C	5.34	1.58	1.52
1	B	318	ASN	CA-C	5.31	1.58	1.52
1	D	210	ILE	CA-C	5.29	1.57	1.53
1	D	174	ALA	N-CA	5.23	1.52	1.46
1	C	34	LEU	N-CA	5.19	1.52	1.46
1	C	354	MET	CA-C	5.10	1.59	1.52
1	B	292	LYS	CA-C	5.07	1.59	1.52
1	D	31	ASP	CA-C	5.07	1.58	1.52
1	A	104	LEU	C-O	-5.00	1.18	1.24

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	292	LYS	N-CA-C	12.27	128.02	113.18
1	B	174	ALA	CA-C-N	7.53	131.44	120.82
1	B	174	ALA	C-N-CA	7.53	131.44	120.82
1	B	285	GLU	N-CA-CB	-7.20	100.00	110.87
1	B	285	GLU	N-CA-C	6.87	119.58	109.69
1	A	292	LYS	N-CA-C	6.13	118.76	111.71
1	B	102	TYR	N-CA-C	6.07	117.90	111.28
1	D	263	THR	N-CA-C	6.03	120.26	113.02
1	D	389	ILE	N-CA-C	5.84	116.03	110.42
1	A	467	ARG	NE-CZ-NH2	5.83	124.45	119.20
1	C	292	LYS	N-CA-C	5.80	119.97	113.01
1	A	308	TYR	N-CA-C	5.69	116.91	108.60
1	A	166	LYS	N-CA-C	5.65	119.99	113.38
1	B	472	ARG	N-CA-C	5.62	115.96	108.38
1	D	292	LYS	N-CA-C	5.37	119.45	113.01
1	D	285	GLU	CA-CB-CG	5.36	124.82	114.10
1	C	314	LEU	CA-C-N	-5.29	114.53	120.14
1	C	314	LEU	C-N-CA	-5.29	114.53	120.14
1	A	482	GLU	N-CA-C	5.25	117.08	111.36
1	B	286	MET	N-CA-C	5.12	118.62	112.38
1	A	472	ARG	N-CA-C	5.08	115.87	108.14

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3976	0	3954	14	0
1	B	3941	0	3903	11	0
1	C	3951	0	3907	19	0
1	D	3931	0	3906	18	0
2	A	36	0	28	5	0
2	B	36	0	26	7	0
2	C	36	0	28	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	36	0	28	4	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	2	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	A	323	0	0	1	0
5	B	317	0	0	1	0
5	C	356	0	0	3	0
5	D	249	0	0	2	0
All	All	17196	0	15780	78	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (78) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:601:4LU:H5	2:D:601:4LU:H14	1.51	0.92
2:B:601:4LU:H14	2:B:601:4LU:H5	1.53	0.91
2:A:601:4LU:H5	2:A:601:4LU:H14	1.55	0.86
2:C:601:4LU:H14	2:C:601:4LU:H5	1.62	0.80
1:C:498:LYS:CA	5:C:1002:HOH:O	2.31	0.77
1:C:322:CYS:H	1:C:359:GLN:HE22	1.34	0.75
1:A:428:VAL:H	1:A:431:GLN:HE21	1.37	0.73
1:A:81:HIS:HE1	1:A:356:TYR:OH	1.77	0.67
1:D:81:HIS:HE1	1:D:356:TYR:OH	1.77	0.66
2:D:601:4LU:H5	2:D:601:4LU:C7M	2.26	0.64
2:B:601:4LU:H14	2:B:601:4LU:C13	2.31	0.60
2:C:601:4LU:H5	2:C:601:4LU:C7M	2.32	0.60
1:C:145:HIS:HE1	1:C:319:PRO:O	1.85	0.59
2:A:601:4LU:H14	2:A:601:4LU:C13	2.32	0.58
1:C:134:ILE:HD12	1:C:306[B]:MET:HE3	1.86	0.58
2:A:601:4LU:H5	2:A:601:4LU:C7M	2.32	0.58
1:D:133:LYS:HA	1:D:133:LYS:CE	2.33	0.58
1:C:268:PHE:CE2	1:C:306[B]:MET:HE2	2.39	0.57
1:B:81:HIS:HE1	1:B:356:TYR:OH	1.87	0.57
1:A:71:ALA:HB3	1:A:325:GLU:HG3	1.86	0.56
1:C:81:HIS:HE1	1:C:356:TYR:OH	1.89	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:428:VAL:H	1:C:431:GLN:HE21	1.51	0.56
1:D:71:ALA:HB3	1:D:325:GLU:HG3	1.87	0.56
1:D:133:LYS:HA	1:D:133:LYS:HE3	1.88	0.56
1:B:428:VAL:H	1:B:431:GLN:HE21	1.54	0.55
1:D:428:VAL:H	1:D:431:GLN:HE21	1.53	0.55
2:D:601:4LU:H14	2:D:601:4LU:C13	2.31	0.54
1:B:145:HIS:HE1	1:B:319:PRO:O	1.92	0.53
2:D:601:4LU:C7M	2:D:601:4LU:C13	2.86	0.53
1:A:12:ASP:O	1:A:16[B]:VAL:HG13	2.09	0.52
1:A:145:HIS:HE1	1:A:319:PRO:O	1.93	0.52
1:D:428:VAL:H	1:D:431:GLN:NE2	2.07	0.52
2:A:601:4LU:C13	2:A:601:4LU:C7M	2.88	0.51
1:C:208[A]:ASN:ND2	1:C:273:SER:OG	2.43	0.51
1:A:436[B]:ASP:OD1	1:A:436[B]:ASP:C	2.54	0.50
1:D:145:HIS:HD2	1:D:148:ASP:OD2	1.94	0.50
1:D:322:CYS:H	1:D:359:GLN:HE22	1.60	0.49
1:C:268:PHE:CD2	1:C:306[B]:MET:HE2	2.47	0.49
1:C:127:HIS:HE1	1:C:310:ASP:OD1	1.95	0.49
2:B:601:4LU:C13	2:B:601:4LU:C7M	2.91	0.48
2:B:601:4LU:H5	2:B:601:4LU:C7M	2.34	0.48
1:C:467:ARG:HD3	5:C:859:HOH:O	2.13	0.48
1:A:134:ILE:HD13	1:A:306[B]:MET:HE3	1.96	0.48
1:B:293:SER:HB2	5:B:964:HOH:O	2.14	0.47
1:C:428:VAL:H	1:C:431:GLN:NE2	2.11	0.47
1:C:137:GLN:NE2	5:C:711:HOH:O	2.49	0.46
2:C:601:4LU:C7M	2:C:601:4LU:C13	2.93	0.46
1:D:145:HIS:CE1	1:D:318:ASN:OD1	2.69	0.45
1:D:279:LEU:HD22	5:D:865:HOH:O	2.16	0.45
1:C:96[A]:ILE:O	1:C:96[A]:ILE:HG13	2.17	0.45
1:C:285:GLU:HG2	1:C:286:MET:N	2.31	0.45
1:A:428:VAL:H	1:A:431:GLN:NE2	2.10	0.45
1:C:145:HIS:HD2	1:C:148:ASP:OD2	2.00	0.44
1:C:4:LEU:HD13	1:C:16[B]:VAL:HG12	2.00	0.44
1:D:387:GLY:HA3	1:D:434:PHE:CZ	2.53	0.43
1:D:127:HIS:HE1	1:D:310:ASP:OD1	2.01	0.43
1:D:198:ALA:HB1	1:D:274:LEU:HD11	1.99	0.43
1:C:146:VAL:O	1:C:147:SER:HB2	2.18	0.43
1:A:145:HIS:HD2	1:A:148:ASP:OD2	2.02	0.43
1:A:188:VAL:O	1:A:195:ARG:HD3	2.19	0.42
1:A:292:LYS:O	1:A:293:SER:C	2.62	0.42
1:D:80:ASP:OD1	1:D:81:HIS:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:489:LEU:HD11	1:B:35:GLU:HG3	2.00	0.42
1:D:145:HIS:HE1	1:D:319:PRO:O	2.01	0.42
2:A:601:4LU:H16	2:A:601:4LU:H17	1.87	0.42
1:B:71:ALA:HB3	1:B:325:GLU:HG3	2.00	0.42
1:B:173:ILE:HD12	2:B:601:4LU:H18	2.01	0.42
1:C:134:ILE:CD1	1:C:306[B]:MET:HE3	2.49	0.42
1:A:436[B]:ASP:OD1	1:A:436[B]:ASP:O	2.36	0.42
1:B:69:CYS:N	1:B:70:PRO:CD	2.82	0.41
1:B:16[A]:VAL:O	1:B:16[A]:VAL:HG22	2.19	0.41
1:A:370[B]:LYS:HG2	5:A:890:HOH:O	2.21	0.41
2:B:601:4LU:H7	2:B:601:4LU:H22	1.84	0.41
1:B:330:ILE:HD11	2:B:601:4LU:C9A	2.51	0.41
1:B:12:ASP:O	1:B:16[B]:VAL:HG13	2.20	0.41
1:D:133:LYS:HA	1:D:133:LYS:HE2	2.02	0.41
1:D:190:LYS:HD3	5:D:841:HOH:O	2.21	0.41
1:D:270:GLY:HA3	1:D:302:THR:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	507/509 (100%)	492 (97%)	15 (3%)	0	100	100
1	B	504/509 (99%)	492 (98%)	12 (2%)	0	100	100
1	C	508/509 (100%)	495 (97%)	13 (3%)	0	100	100
1	D	501/509 (98%)	487 (97%)	14 (3%)	0	100	100
All	All	2020/2036 (99%)	1966 (97%)	54 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	440/443 (99%)	433 (98%)	7 (2%)	55	56
1	B	435/443 (98%)	426 (98%)	9 (2%)	47	46
1	C	436/443 (98%)	427 (98%)	9 (2%)	47	46
1	D	435/443 (98%)	422 (97%)	13 (3%)	36	32
All	All	1746/1772 (98%)	1708 (98%)	38 (2%)	47	44

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	93	LYS
1	A	133	LYS
1	A	137	GLN
1	A	181	ASP
1	A	285	GLU
1	A	473[A]	SER
1	A	473[B]	SER
1	B	108	GLU
1	B	119	VAL
1	B	137	GLN
1	B	190	LYS
1	B	269	GLU
1	B	279	LEU
1	B	285	GLU
1	B	460	CYS
1	B	471	GLU
1	C	132	GLU
1	C	137	GLN
1	C	167	LYS
1	C	220	PRO
1	C	269	GLU
1	C	285	GLU
1	C	380	GLU
1	C	460[A]	CYS

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Mol	Chain	Res	Type
1	C	460[B]	CYS
1	D	110	GLU
1	D	132	GLU
1	D	133	LYS
1	D	137	GLN
1	D	181	ASP
1	D	190	LYS
1	D	220	PRO
1	D	269	GLU
1	D	279	LEU
1	D	285	GLU
1	D	292	LYS
1	D	460[A]	CYS
1	D	460[B]	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	81	HIS
1	A	127	HIS
1	A	145	HIS
1	A	162	GLN
1	A	193	HIS
1	A	373	GLN
1	A	431	GLN
1	A	448	GLN
1	B	33	ASN
1	B	81	HIS
1	B	127	HIS
1	B	145	HIS
1	B	162	GLN
1	B	431	GLN
1	B	469	GLN
1	C	33	ASN
1	C	81	HIS
1	C	127	HIS
1	C	145	HIS
1	C	359	GLN
1	C	431	GLN
1	D	15	GLN
1	D	81	HIS

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Mol	Chain	Res	Type
1	D	127	HIS
1	D	137	GLN
1	D	145	HIS
1	D	311	ASN
1	D	359	GLN
1	D	431	GLN
1	D	448	GLN
1	D	496	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	4LU	C	601	4,3	35,39,39	1.67	4 (11%)	44,62,62	2.03	13 (29%)
2	4LU	B	601	4,3	35,39,39	3.20	8 (22%)	44,62,62	2.30	16 (36%)
2	4LU	A	601	4,3	35,39,39	1.79	6 (17%)	44,62,62	1.89	13 (29%)
2	4LU	D	601	3	35,39,39	1.68	3 (8%)	44,62,62	2.18	16 (36%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	4LU	C	601	4,3	-	1/18/30/30	0/4/4/4
2	4LU	B	601	4,3	-	2/18/30/30	0/4/4/4
2	4LU	A	601	4,3	-	2/18/30/30	0/4/4/4
2	4LU	D	601	3	-	2/18/30/30	0/4/4/4

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	4LU	C1'-N10	-15.58	1.10	1.47
2	D	601	4LU	O2-C2	6.29	1.36	1.23
2	B	601	4LU	O2-C2	5.82	1.35	1.23
2	C	601	4LU	O2-C2	5.79	1.35	1.23
2	A	601	4LU	O2-C2	5.72	1.35	1.23
2	A	601	4LU	C3-C5	-5.32	1.46	1.54
2	C	601	4LU	C3-C5	-4.91	1.46	1.54
2	B	601	4LU	C1'-C2'	4.32	1.58	1.52
2	D	601	4LU	C3-C5	-4.05	1.48	1.54
2	B	601	4LU	C3-C5	-3.93	1.48	1.54
2	A	601	4LU	C9-C8	-2.89	1.35	1.39
2	B	601	4LU	C5A-C6	2.84	1.42	1.39
2	B	601	4LU	C10-N10	2.64	1.43	1.38
2	D	601	4LU	C5'-C4'	2.60	1.55	1.51
2	B	601	4LU	C8M-C8	-2.58	1.46	1.51
2	C	601	4LU	C10-N10	2.36	1.42	1.38
2	C	601	4LU	P-O3P	-2.33	1.46	1.54
2	A	601	4LU	O4-C4	2.24	1.27	1.23
2	A	601	4LU	C4'-C3'	-2.08	1.49	1.53
2	B	601	4LU	C5'-C4'	2.08	1.54	1.51
2	A	601	4LU	C8M-C8	-2.07	1.47	1.51

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	4LU	C5-C6-C5A	-6.12	114.80	121.48
2	C	601	4LU	C5-C6-C5A	-5.54	115.43	121.48
2	B	601	4LU	C5-C6-C5A	-5.48	115.50	121.48
2	B	601	4LU	C2'-C1'-N10	5.27	135.11	110.20
2	B	601	4LU	C1'-C2'-C3'	5.16	123.64	109.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	4LU	C4A-C4-N3	4.93	122.04	111.84
2	C	601	4LU	C4A-C4-N3	4.90	121.98	111.84
2	D	601	4LU	C4A-C4-N3	4.54	121.22	111.84
2	D	601	4LU	C4-N3-C2	-4.44	120.25	126.37
2	C	601	4LU	C13-C5-C3	-4.34	102.81	109.50
2	A	601	4LU	N1-C2-N3	4.21	122.35	115.74
2	B	601	4LU	C4-N3-C2	-4.12	120.70	126.37
2	A	601	4LU	C9-C8-C7	4.04	123.17	119.10
2	A	601	4LU	C5-C6-C5A	-3.82	117.31	121.48
2	C	601	4LU	C4-N3-C2	-3.71	121.27	126.37
2	D	601	4LU	C13-C5-C3	-3.55	104.03	109.50
2	A	601	4LU	C4A-C4-N3	3.46	119.00	111.84
2	D	601	4LU	C8M-C8-C7	3.45	126.05	121.18
2	A	601	4LU	C4-N3-C2	-3.30	121.83	126.37
2	D	601	4LU	O1P-P-O5'	3.28	115.23	106.67
2	D	601	4LU	C8M-C8-C9	-3.25	113.85	119.57
2	D	601	4LU	C2'-C1'-N10	3.23	125.48	110.20
2	C	601	4LU	O4-C4-N3	-3.10	114.28	120.11
2	D	601	4LU	C4'-C3'-C2'	-3.06	108.47	113.57
2	B	601	4LU	C13-C5-C3	-3.01	104.86	109.50
2	A	601	4LU	C8M-C8-C9	-2.95	114.37	119.57
2	B	601	4LU	O5'-P-O2P	-2.77	98.95	106.44
2	B	601	4LU	C9-C8-C7	2.77	121.89	119.10
2	C	601	4LU	C8M-C8-C9	-2.76	114.71	119.57
2	B	601	4LU	C4'-C3'-C2'	2.74	118.12	113.57
2	A	601	4LU	C2'-C1'-N10	2.71	123.03	110.20
2	C	601	4LU	C9-C8-C7	2.69	121.81	119.10
2	B	601	4LU	O4-C4-N3	-2.69	115.06	120.11
2	A	601	4LU	C1'-N10-C9A	2.68	125.85	120.63
2	D	601	4LU	O1P-P-O3P	2.67	117.81	107.80
2	D	601	4LU	C3-C5-C6	2.67	113.47	107.38
2	D	601	4LU	C12-C5-C3	-2.65	105.41	109.50
2	C	601	4LU	N1-C2-N3	2.65	119.91	115.74
2	A	601	4LU	O1P-P-O3P	2.64	117.71	107.80
2	B	601	4LU	O2'-C2'-C3'	-2.64	103.08	109.25
2	A	601	4LU	C13-C5-C3	-2.63	105.44	109.50
2	C	601	4LU	C2'-C1'-N10	2.60	122.48	110.20
2	B	601	4LU	O1P-P-O3P	2.50	117.17	107.80
2	D	601	4LU	O4-C4-N3	-2.48	115.44	120.11
2	C	601	4LU	O1P-P-O3P	2.45	116.97	107.80
2	B	601	4LU	C1'-N10-C9A	2.44	125.38	120.63
2	D	601	4LU	N1-C2-N3	2.37	119.47	115.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	4LU	O4-C4-C4A	-2.32	122.83	128.01
2	A	601	4LU	O4-C4-N3	-2.26	115.86	120.11
2	C	601	4LU	C7M-C7-C8	-2.19	115.89	119.67
2	B	601	4LU	C12-C5-C3	-2.18	106.14	109.50
2	D	601	4LU	O5'-P-O2P	-2.14	100.66	106.44
2	A	601	4LU	O3P-P-O5'	-2.11	101.16	106.67
2	D	601	4LU	O4-C4-C4A	-2.10	123.33	128.01
2	A	601	4LU	O2-C2-N3	-2.09	118.14	121.86
2	B	601	4LU	C8M-C8-C9	-2.09	115.88	119.57
2	C	601	4LU	O5'-C5'-C4'	-2.07	103.84	109.36
2	C	601	4LU	C1'-N10-C9A	2.05	124.61	120.63

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	4LU	C2'-C3'-C4'-C5'
2	B	601	4LU	C2'-C3'-C4'-C5'
2	A	601	4LU	C4'-C5'-O5'-P
2	D	601	4LU	C4'-C5'-O5'-P
2	C	601	4LU	C2'-C3'-C4'-C5'
2	B	601	4LU	C4'-C5'-O5'-P
2	D	601	4LU	C2'-C3'-C4'-C5'

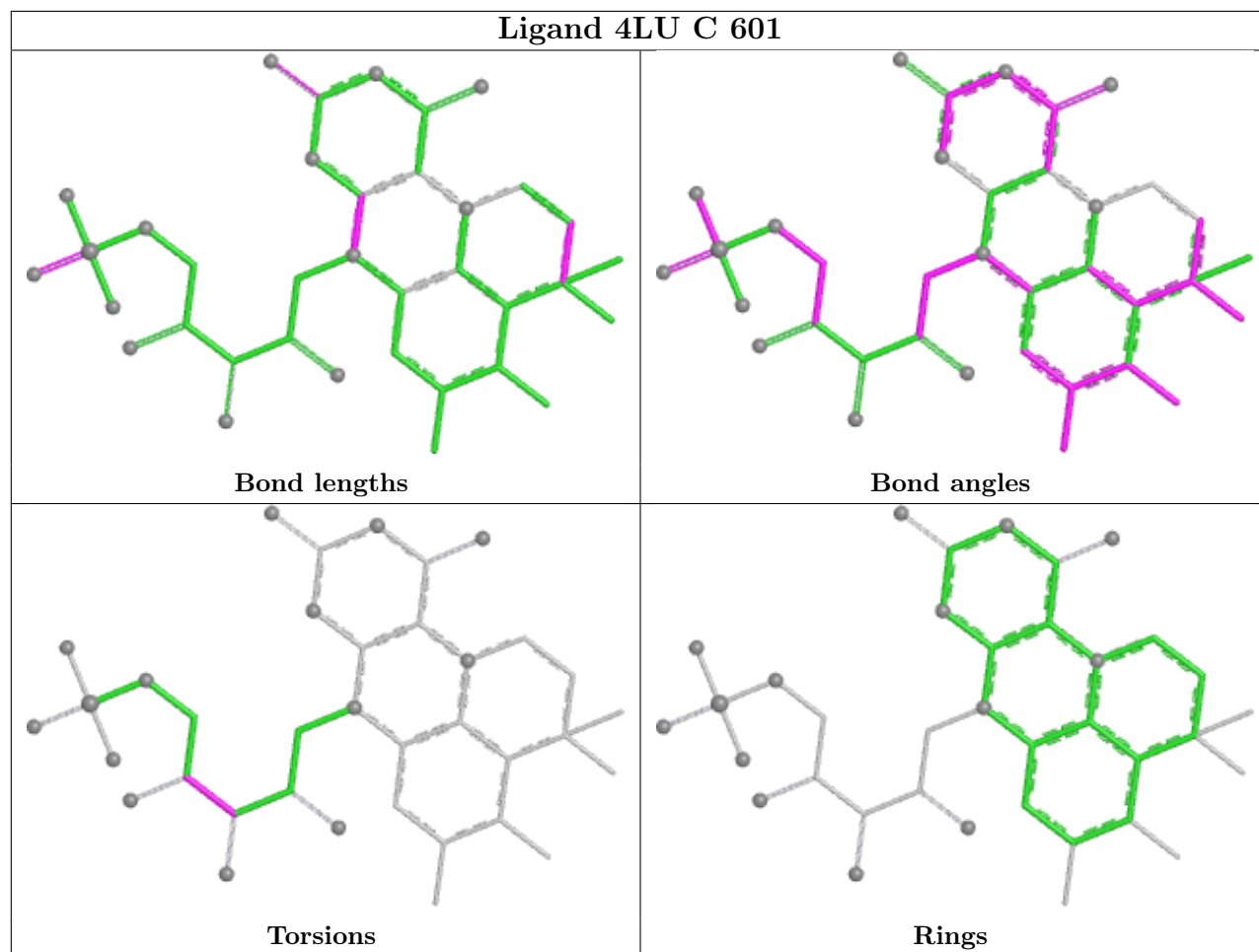
There are no ring outliers.

4 monomers are involved in 19 short contacts:

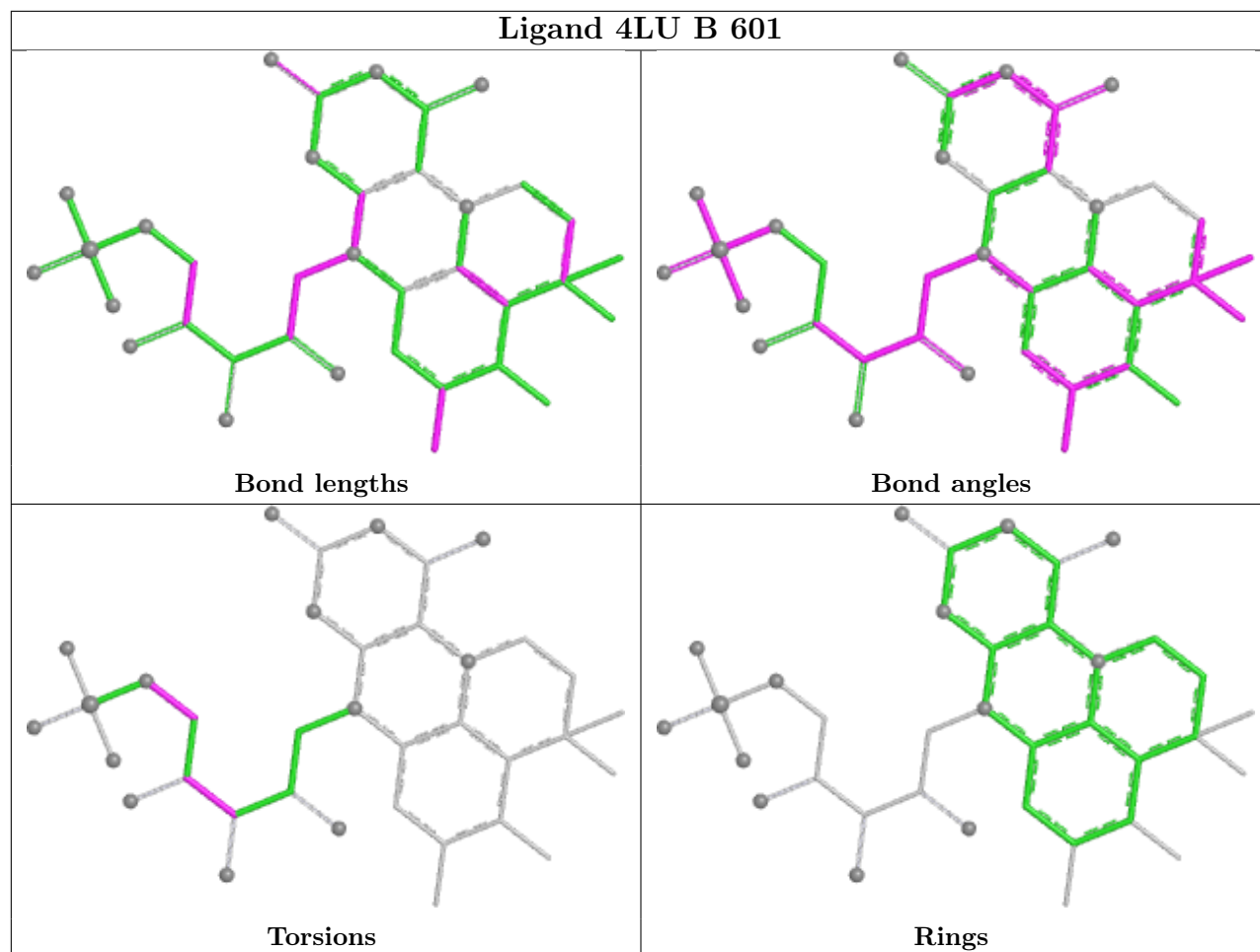
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	601	4LU	3	0
2	B	601	4LU	7	0
2	A	601	4LU	5	0
2	D	601	4LU	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

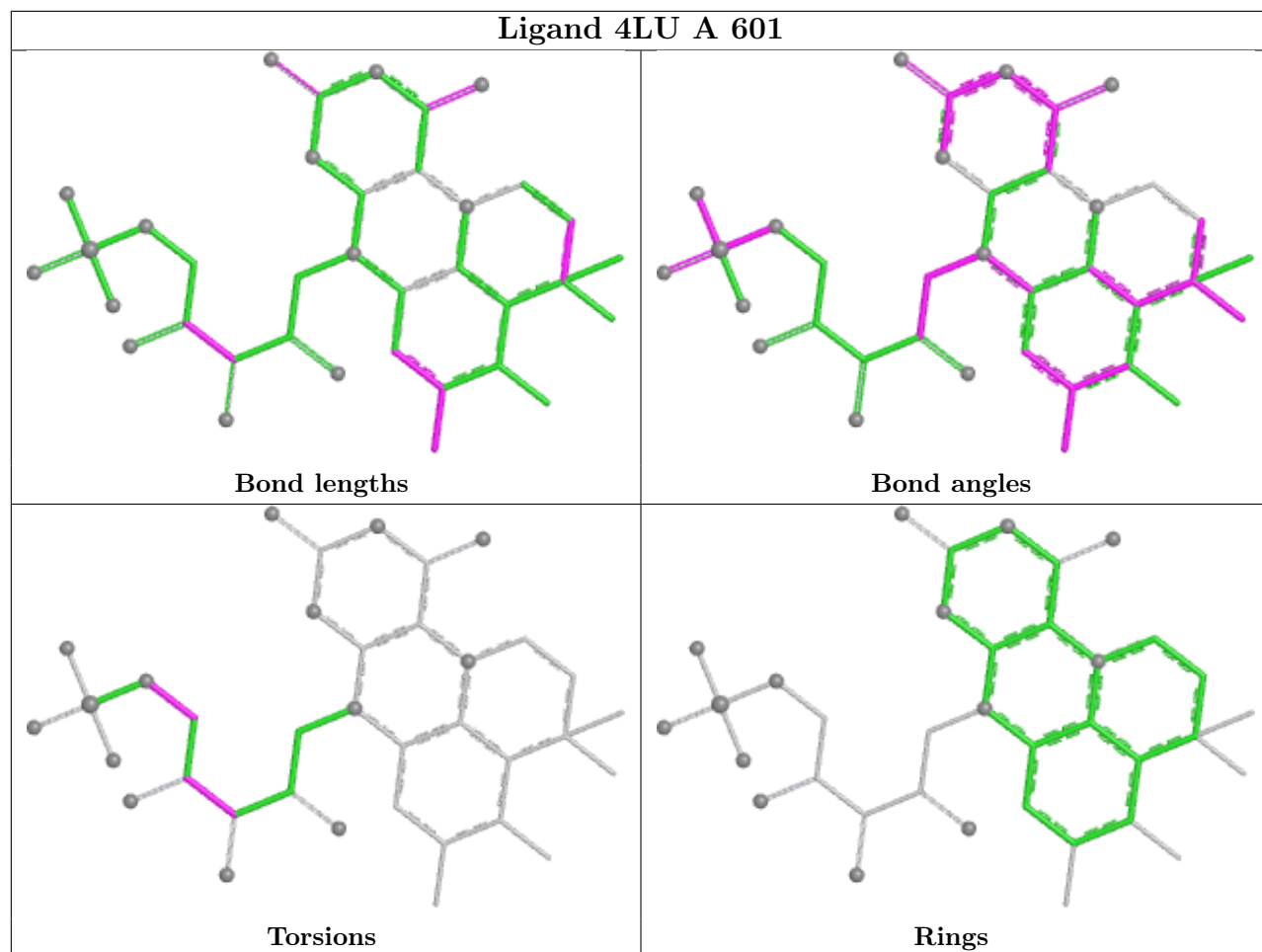
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

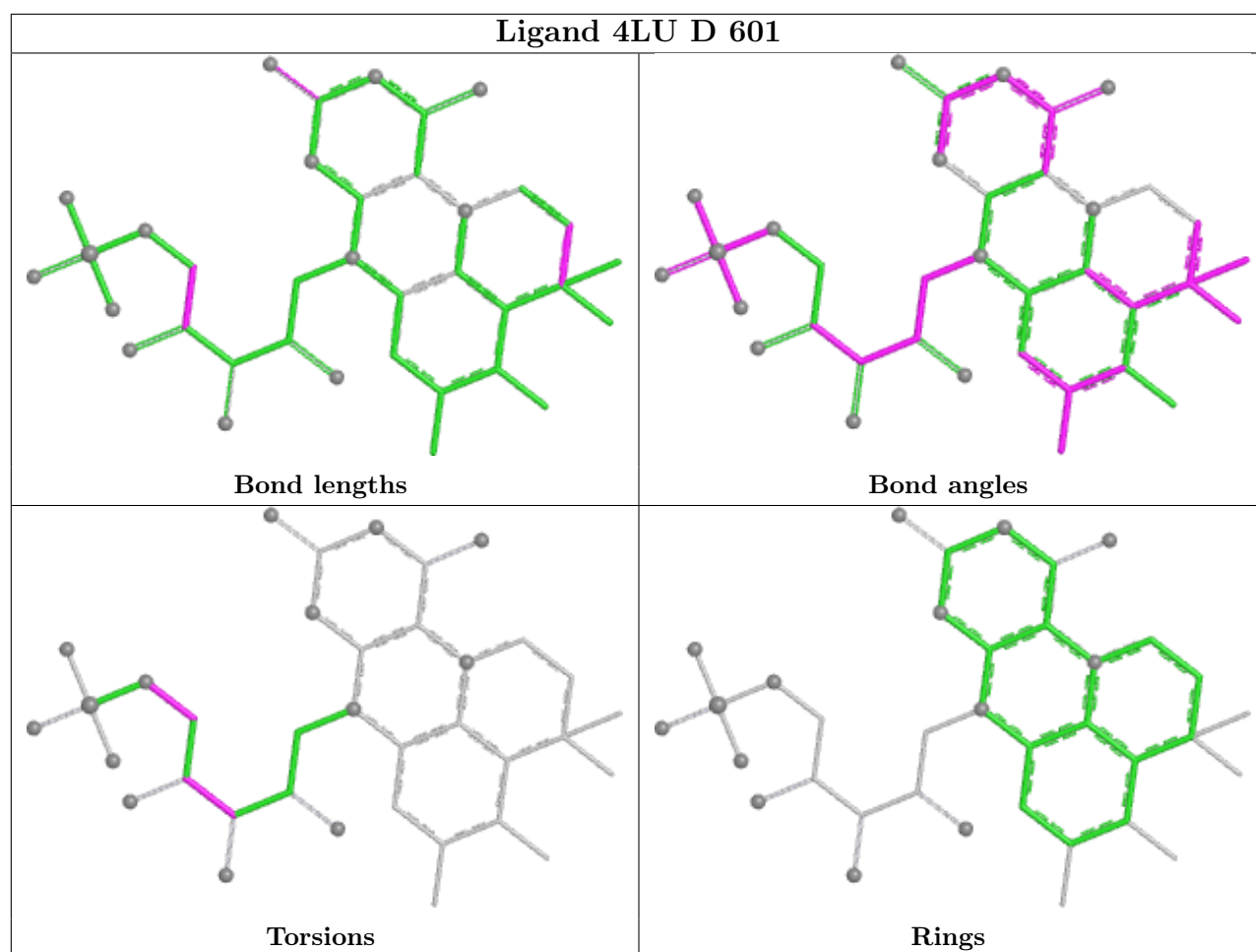


Ligand 4LU B 601



Ligand 4LU A 601





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	500/509 (98%)	-0.46	3 (0%) 85 87	8, 23, 39, 57	11 (2%)
1	B	499/509 (98%)	-0.31	7 (1%) 73 75	11, 26, 44, 65	9 (1%)
1	C	500/509 (98%)	-0.29	3 (0%) 85 87	10, 25, 43, 58	12 (2%)
1	D	497/509 (97%)	-0.22	4 (0%) 82 84	10, 28, 43, 64	9 (1%)
All	All	1996/2036 (98%)	-0.32	17 (0%) 81 83	8, 25, 43, 65	41 (2%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	294	GLN	9.4
1	C	296	HIS	6.6
1	D	4[A]	LEU	4.5
1	D	297	PRO	3.1
1	B	473[A]	SER	3.0
1	B	503	LYS	3.0
1	C	295	GLY	2.4
1	B	293	SER	2.4
1	D	293	SER	2.4
1	B	292	LYS	2.4
1	A	293	SER	2.2
1	B	455	MET	2.2
1	B	297	PRO	2.1
1	B	2	ARG	2.1
1	D	292	LYS	2.1
1	A	297	PRO	2.1
1	A	455	MET	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

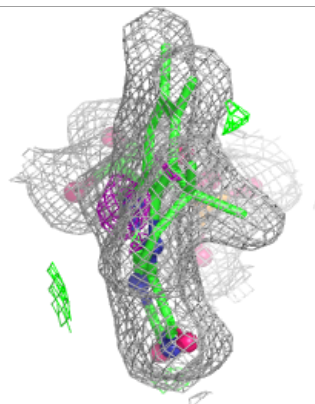
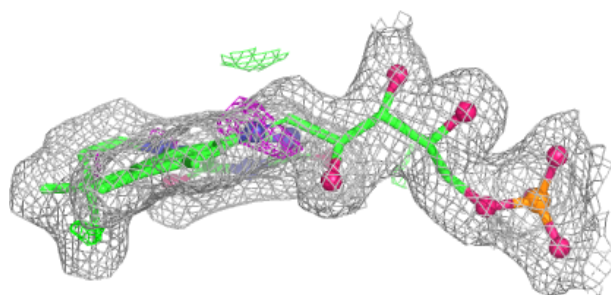
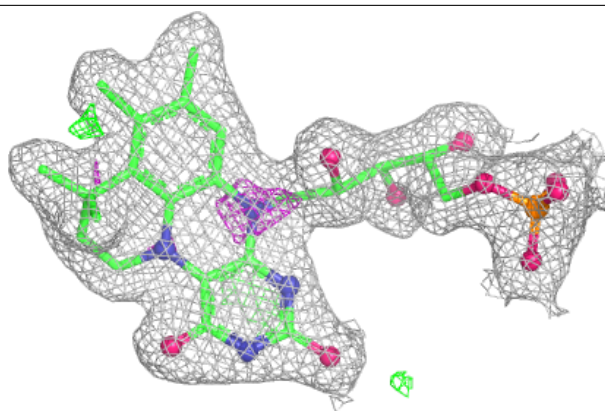
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	4LU	B	601	36/36	0.96	0.07	15,18,22,25	0
2	4LU	A	601	36/36	0.98	0.05	15,17,22,28	0
2	4LU	C	601	36/36	0.98	0.05	15,20,27,31	0
2	4LU	D	601	36/36	0.98	0.05	16,22,25,26	0
3	MN	C	602	1/1	0.99	0.03	24,24,24,24	0
3	MN	D	602	1/1	0.99	0.03	24,24,24,24	0
3	MN	D	603	1/1	0.99	0.09	32,32,32,32	0
4	K	A	603	1/1	0.99	0.03	18,18,18,18	0
4	K	B	603	1/1	0.99	0.04	21,21,21,21	0
3	MN	B	602	1/1	1.00	0.02	27,27,27,27	0
3	MN	A	602	1/1	1.00	0.03	24,24,24,24	0
4	K	C	603	1/1	1.00	0.04	19,19,19,19	0

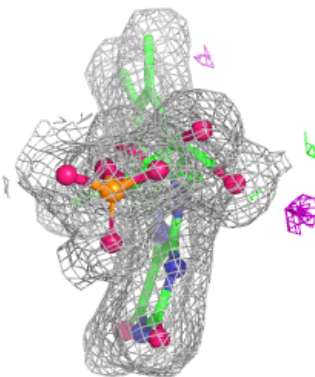
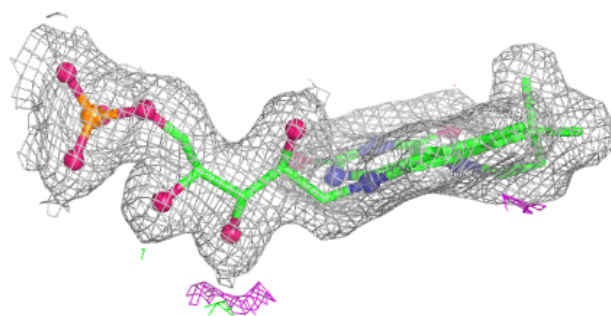
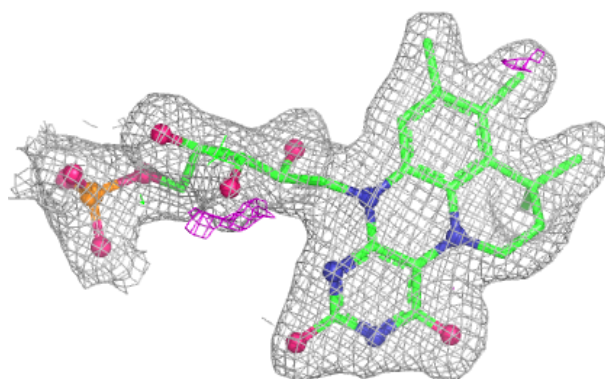
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 4LU B 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

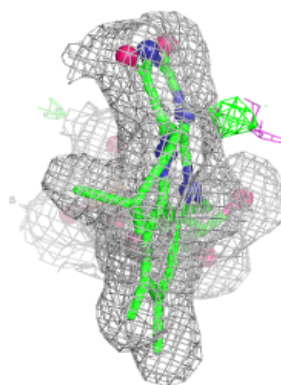
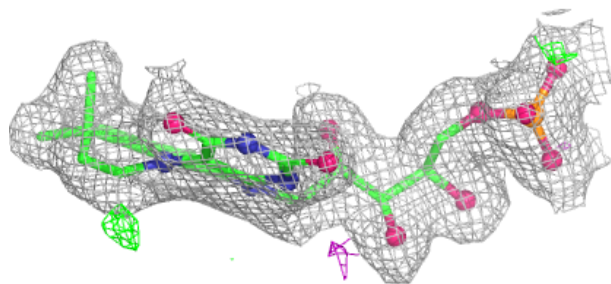
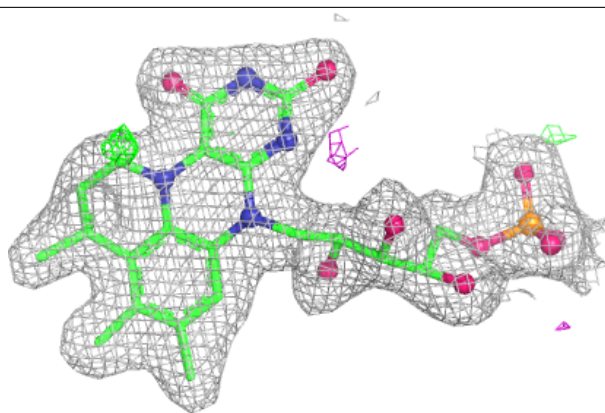
**Electron density around 4LU A 601:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

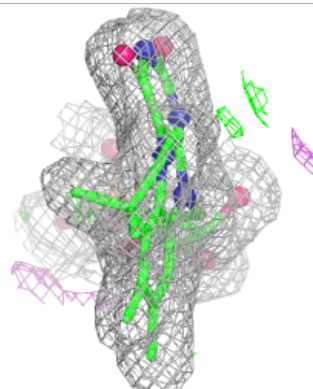
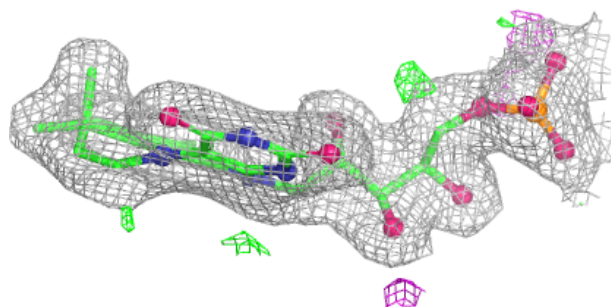
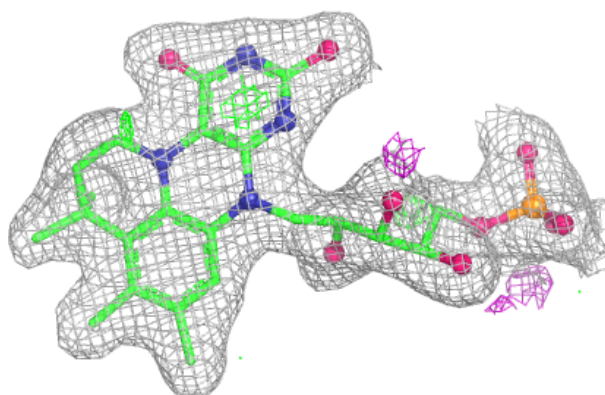


Electron density around 4LU C 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around 4LU D 601:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.